

On the tritium β - electrons energy shape

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Abstract

A series of high precision atomic experiments was carried out last decade to get a better estimate for the electron (anti) neutrino mass m_ν . The reaction to be observed is molecular tritium β - decay. The m_ν value serves as one of the tune parameters to fit β - electrons spectrum via reference theoretical one. The unexpected message consists of that parameter m_ν^2 has to be fixed at some negative value to get best statistically reliable fit. Apart of some exotic scenarios suggested the problem remains open. In this paper we tried to reanalyze ground features of the final states spectrum (FSS) and its influence on the β - electrons spectrum. A new approach has been developed which gives some hints to make proper modifications to the tabulated FSS in the course of experimental fits.

I. INTRODUCTION

The last atomic neutrino experiments base on the observation of molecular tritium β - decay [1] :

$$T_2 \rightarrow T^3He^+ + e^- + \tilde{\nu}_e \quad (1)$$

The high energy edge of β - electrons spectrum corresponds to about 18.6 KeV. The sudden change of the nuclear charge and hard recoil kick lead to the population of the hundreds

electronic- rovibrational states of final T^3He^+ molecule. The neutrinos $\tilde{\nu}_e$ are hardly observable but they influence total energy sharing and consequently β - electrons energy spectrum.

The β - electrons differential energy spectrum can be written in the following form [2]:

$$\left| \frac{dN(\epsilon_\beta)}{d\epsilon_\beta} \right| = AF(p_\beta, Z)E_\beta p_\beta \sum_n P_n(p_\beta) \epsilon_n (\epsilon_n^2 - m_\nu^2 c^4)^{1/2} \theta(\epsilon_n - m_\nu c^2), \quad (2)$$

$$\epsilon_n = W_0 - \epsilon_\beta - E_n, \epsilon_\beta = E_\beta - m_e c^2.$$

The sum in (2) runs over final states of T^3He^+ molecule; E_β, ϵ_β are the total relativistic- and kinetic energies and p_β is the momentum of β -electrons; $F(p_\beta, Z)$ is the so called Fermi factor which takes into account Coulomb charge Z of the daughter nucleus [3]. If we will count final energies E_n from the ground E_g state of T^3He^+ , the end-point β -electron kinetic energy W_0 is given by the relation:

$$W_0 = (M_t - M_\alpha)c^2 + E_{T_2} - E_g - E_R - m_e c^2, \quad (3)$$

where E_{T_2} is the ground state of parent T_2 molecule; $E_R = \frac{p_\beta^2}{4M_t}$ is the molecular center of mass recoil energy. The final states population probabilities $P_n(p_\beta)$ are given by the corresponding matrix elements:

$$P_n(p_\beta) = \int \frac{d\hat{\mathbf{q}}}{4\pi} | \langle n | e^{i(\mathbf{q}, \mathbf{R})} | T_2 \rangle |^2, \quad \mathbf{q} = \frac{\mathbf{p}_\beta}{2}, \quad (4)$$

where \mathbf{R} is the internuclear distance [5]. The β - spectrometers currently operating in Mainz and Troitsk detect actually integral spectrum for which we have :

$$N(\epsilon_\beta) = \frac{A}{3} F(p_\beta, Z) E_\beta p_\beta \sum_n P_n(p_\beta) (\epsilon_n^2 - m_\nu^2 c^4)^{3/2} \theta(\epsilon_n - m_\nu c^2). \quad (5)$$

The standard procedure consists of fitting experimental spectrum close to the end-point energy W_0 using formula (5) varying three parameters A, E_0, m_ν^2 and value of background.

Since first quantitative results have been published in the literature, immense work has been done to purify theoretical spectrum in many different aspects [4]. They showed that about 99% of final states spectrum covers over 100 eV. It mostly consists of the several eV narrow rovibrational multiplets wired on bound and resonance adiabatic electronic states as

it is shown in Fig. 1. Some 57% falls on to electronic ground state of T^3He^+ . The rovibrational multiplet consists of hundreds bound and resonance states distributed "...unevenly in a somewhat erratic manner" with average rotational quantum number $J \sim 22 \div 25$ [2]. The reason is a huge, on the atomic scale, recoil momentum $q \sim 18$ releasing.

The results of extensive joint fits between experiments and available theoretical tables show with a certainty that parameter m_ν^2 should be set at a *negative* value. The definite value explicitly depends on the chosen energy fit interval. Though physically unsatisfactory, it permits to draw up an upper estimate $m_\nu \leq 2 \div 3 \text{ eV}/c^2$.

The critical values of $m_\nu \sim 1 \text{ eV}/c^2$ will be decisive, e.g. for "dark matter" problem. The series of experiments aiming to hit this border are on the list of Mainz-Troitsk collaboration. The "negative m_ν^2 " problem will represent then one of the serious bottlenecks. To exclude reasons related to the FSS we went to reanalyze basic issues in the theoretical final states spectrum and its influence on the β -electrons spectrum.

II. β -SPECTRUM: GENERAL FEATURES.

As Eqs.(2), (5) suggest, the sign of non-zero neutrino mass is the non-analytic behavior close to the branch energy of given channel. We would like to show, however, that a somewhat simpler functional form is enough for all practical purposes. Let us take for granted that m_ν^2 is a small parameter:

$$\epsilon_n^3 - m_\nu^2 c^4 \epsilon_n + O\left(\left|\frac{(m_\nu^2 c^4)^2}{\epsilon_n}\right|\right), \quad (6)$$

which gives for the spectral sum itself:

$$\sum_n P_n(p_\beta) [\epsilon_n^3 - m_\nu^2 c^4 \epsilon_n] \theta(\epsilon_n - m_\nu c^2). \quad (7)$$

We can further expand θ -function

$$\theta(\epsilon_n - m_\nu c^2) = \theta(\epsilon_n) - \delta(\epsilon_n) m_\nu c^2 + \dots \quad (8)$$

to show that neutrino mass term enters into the spectrum, essentially, via linear energy term (7). We plot in Fig. 2 absolute difference between spectral sum in (5) and its linear approximation (7) using FSS from [2]. It shows that absolute difference is uniformly bounded and decreases roughly as $(m_\nu c^2)^4/(W_0 - \epsilon_\beta)$. The formula (7) can be further transformed to the particularly transparent form:

$$P_\epsilon \left[\epsilon^3 - 3 \langle E_n \rangle_\epsilon \epsilon^2 + 3 \langle E_n^2 \rangle_\epsilon \epsilon - \frac{3}{2} m_\nu^2 c^4 (\epsilon - \langle E_n \rangle_\epsilon) - \langle E_n^3 \rangle_\epsilon \right], \quad (9)$$

where we introduced FSS cumulative momenta

$$P_\epsilon = \sum_n \theta(\epsilon_n), \quad \langle E_n \rangle_\epsilon = 1/P_\epsilon \sum_n E_n \theta(\epsilon_n) \dots$$

It shows that β -spectrum can be parametrised using few statistical characteristics of the full FSS.

III. β -SPECTRUM: OPERATOR FORMULATION.

To find some way to calculate cumulative momenta directly, we use in (2) well-known substitution $E_n \rightarrow H$, where H is Hamiltonian of T^3He^+ molecule. Completing the sum over final spectrum, we get:

$$N(\epsilon_\beta) = \frac{A}{3} F(p_\beta, Z) E_\beta p_\beta \int \frac{d\mathbf{q}}{4\pi} \langle T_2 | e^{-i(\mathbf{q}, \mathbf{R})} \left(\epsilon^2 - m_\nu^2 c^4 \right)^{3/2} \theta(W_0 - \epsilon_\beta - H) e^{i(\mathbf{q}, \mathbf{R})} | T_2 \rangle, \quad (10)$$

here $\epsilon = W_0 - \epsilon_\beta - H$. It is easy to justify the following commutation relation:

$$H e^{i(\mathbf{q}, \mathbf{R})} = e^{i(\mathbf{q}, \mathbf{R})} \left[H + \frac{q^2}{2M} + \frac{(\mathbf{q}, \hat{\mathbf{p}}_{\mathbf{R}})}{M} \right], \quad (11)$$

using explicit form of kinetic energy operator $T_k = -\frac{1}{2M}\Delta$. We can eliminate now recoil exponent, making simultaneous substitution in (10):

$$W_0 - \epsilon_\beta - H \rightarrow W_0 - \epsilon_\beta - \frac{q^2}{2M} - \frac{(\mathbf{q}, \hat{\mathbf{p}}_{\mathbf{R}})}{M} - H \quad (12)$$

The term $\frac{q^2}{2M}$ can be interpreted as an integral rotational recoil energy shift. It adds up to the center-of-mass recoil energy

$$E_R \rightarrow E_R + \frac{q^2}{2M} = \frac{p_\beta^2}{2M_t} = \frac{\epsilon_\beta}{M_t} \left(1 + \frac{\epsilon_\beta}{2m_e c^2}\right). \quad (13)$$

The additional operator term in (12) is estimated at $\left|\frac{(\mathbf{q}, \hat{\mathbf{p}}_{\mathbf{R}})}{M}\right| \sim 10^{-2}$. We will use it like an expansion parameter.

To start with θ -function in (10), we use following relation:

$$f(\hat{A} + \hat{\epsilon}) = f(\hat{A}) + f'(\hat{A})\hat{\epsilon} + \frac{1}{2}f''(\hat{A})[\hat{\epsilon}, \hat{A}] + O(\hat{\epsilon}^2, [\hat{A}, [\hat{\epsilon}, \hat{A}]], \dots)$$

to get

$$\theta(\hat{\epsilon} - \frac{(\mathbf{q}, \hat{\mathbf{p}}_{\mathbf{R}})}{M}) = \theta(\hat{\epsilon}) - \delta(\hat{\epsilon}) \frac{(\mathbf{q}, \hat{\mathbf{p}}_{\mathbf{R}})}{M} + \dots, \quad (14)$$

The general functions must be understood as usually in terms of convolution with smooth-class functions. In our case it is naturally provided by the final energy resolution. The experimentally observed spectra are defined by

$$N_{exp}(\epsilon_\beta) = \int d\epsilon R(\epsilon_\beta - \epsilon) N(\epsilon),$$

where $N(\epsilon)$ is the one from (2). Taking for example generic case of Gaussian

$$R(\epsilon) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\epsilon^2/2\sigma^2},$$

we conclude that δ -like terms in (14) will produce local corrections the type shown in Fig.2. Moreover, due to additional $\int d\hat{\mathbf{q}}$ integration leading order correction will be quadratic in $\left|\frac{(\mathbf{q}, \hat{\mathbf{p}}_{\mathbf{R}})}{M}\right|^2$. Their total spectral power should be sufficiently small, therefor we keep in (14) leading term only.

It is easy to follow that expansion of "3/2"-function over $\frac{(\mathbf{q}, \hat{\mathbf{p}}_{\mathbf{R}})}{M}$ parameter with consequent $\int d\hat{\mathbf{q}}$ average will give:

$$\left(\hat{\epsilon}^2 - m_\nu^2 c^4\right)^{3/2} - \left(\frac{q}{M}\right)^2 \Delta_{\mathbf{R}} \hat{\epsilon} + \hat{C} + O\left(\frac{(m_\nu c^2)^4}{\hat{\epsilon}^2} \left|\frac{(\mathbf{q}, \hat{\mathbf{p}}_{\mathbf{R}})}{M}\right|^2\right). \quad (15)$$

The particular form of \hat{C} depends on the operator order in (15) and is given by

$$\hat{C} = -\frac{1}{3} \left(\frac{q}{M} \right)^2 \left(\left[\left[H, \frac{d}{dR} \right], \frac{d}{dR} \right] - \frac{d}{dR} \left[H, \frac{d}{dR} \right] \right).$$

The spectral power of this term is relative small, e.g. for T^3He^+ electronic ground state we have $|\hat{C}| \leq 0.1 \text{ eV}^3$.

Putting all together we get a new representation for the β -spectrum:

$$N(\epsilon_\beta) = \frac{A}{3} F(p_\beta, Z) E_\beta p_\beta < T_2 | [(\hat{\epsilon}^2 - m_\nu^2 c^4)^{3/2} - \left(\frac{q}{M} \right)^2 \Delta_{\mathbf{R}} \hat{\epsilon} + \hat{C}] \theta(\hat{\epsilon}) | T_2 >. \quad (16)$$

The differential spectrum is written down analogously:

$$\frac{dN(\epsilon_\beta)}{d\epsilon_\beta} = A F(p_\beta, Z) E_\beta p_\beta < T_2 | [\hat{\epsilon} (\hat{\epsilon}^2 - m_\nu^2 c^4)^{1/2} - \frac{1}{3} \left(\frac{q}{M} \right)^2 \Delta_{\mathbf{R}}] \theta(\hat{\epsilon}) | T_2 >. \quad (17)$$

The new final states expansion formula appears after plug-in $\sum_n |n\rangle \langle n| = 1$ into (16), (17). For the integral spectrum we have:

$$\begin{aligned} N(\epsilon_\beta) = \frac{A}{3} F(p_\beta, Z) E_\beta p_\beta \sum_n \tilde{P}_n [(\epsilon_n^2 - m_\nu^2 c^4)^{3/2} - \left(\frac{q}{M} \right)^2 \epsilon_n < T_2 | \Delta_{\mathbf{R}} | n \rangle \langle n | T_2 \rangle / \tilde{P}_n + \\ < T_2 | \hat{C} | n \rangle \langle n | T_2 \rangle / \tilde{P}_n] \theta(\epsilon_n) \quad , \quad \tilde{P}_n = | \langle T_2 | n \rangle |^2. \end{aligned} \quad (18)$$

IV. DISCUSSION

Let us discuss derived formulas. Compare formulas (9) and (16) we get the following operator expressions for the cumulative momenta:

$$\begin{aligned} P_\epsilon = < T_2 | \theta(\hat{\epsilon}) | T_2 > \quad , \quad < E_n >_\epsilon = < T_2 | H \theta(\hat{\epsilon}) | T_2 > / P_\epsilon + \frac{q^2}{2M} \\ < E_n^2 >_\epsilon = [< T_2 | (H + \frac{q^2}{2M})^2 \theta(\hat{\epsilon}) | T_2 > - \left(\frac{q}{M} \right)^2 < T_2 | \Delta_{\mathbf{R}} | T_2 >] / P_\epsilon. \end{aligned} \quad (19)$$

As it follows from (18), the *pseudo*-spectrum of final excitations contains vibrational modes only. The term $\frac{q^2}{2M}$ represents uniform rotational recoil energy shift. Consider as an example T^3He^+ ground electronic state. The pseudo-spectrum of final excitations is emptied by the overlap with the first few vibrational states

$$| \langle T_2 | g, v = 0 \rangle |^2 = 52.2\%, \quad | \langle T_2 | g, v = 1 \rangle |^2 = 4.62\% \\ | \langle T_2 | g, v = 2 \rangle |^2 = 0.45\%, \quad | \langle T_2 | g, v = 3 \rangle |^2 = 0.08\% \dots$$

The total sum, as before, is equal to the integral probability 57.4%. Using calculated population probabilities, we can find electronic ground state first energy moment

$$\langle E_n \rangle_g = \frac{q^2}{2M} + 1/P_g \sum_n \tilde{P}_n E_n = 1.72 + 0.03 = 1.75 \text{ eV}.$$

To get exactly same result one has to sum some hundreds lines in the standard approach. Note that vibrational recoil shift is generally ~ 0.1 eV. The sign of the shift depends on the particular state. As for the first excited electronic state it is negative. In the relation to the highly excited electronic states our approach also give clear recipe on how to incorporate correctly nuclear motion. It will be enough to consider that in the final state nuclei move under effective Coulomb repulsion $Z(\approx 2)/R$.

We would like to discuss now one very interesting consequence of our formulas. We have noted already in the course our derivation that composite center-of-mass, rotational recoil shift is

$$E_R = \frac{\epsilon_\beta}{M_t} \left(1 + \frac{\epsilon_\beta}{2m_e c^2} \right) \approx E_R^0 - \frac{W_0 - \epsilon_\beta}{M_t}.$$

That corresponds to the effective change of the end-point energy W_0 as it is seen at $W_0 - \epsilon_\beta$ below true end-point energy W_0 :

$$W_0^{(eff)} = W_0 - \delta W_0 \quad , \quad \delta W_0 = \frac{W_0 - \epsilon_\beta}{M_t}.$$

One can guess that W_0 fit value will be dominated by the lower energy end, where spectral yield is huge. At ~ 200 eV below end-point energy we have $\delta W_0 \sim 0.04$ eV. This value is comparable with the statistical uncertainty of W_0 . Fixing $W_0^{(eff)}$, we sweep into the W_0 energy region, where small neutrino mass term is comparable with the total spectral yield. To compensate deficit of spectral yield caused by lower value of $W_0^{(eff)}$, we have to make m_ν^2 negative. The rough estimate give us some few eV² of negative shift. The fit experiments have to show real size of the effect.

The integral recoil energy shift is clearly associated with the p_β -dependence of the final states probability distribution $P_n(p_\beta)$. The precise nature of that dependence wasn't available, apart the fact that $P_n(p_\beta)$ change wildly at small variations of $q(p_\beta)$.

Last notes concern of the other possible experimental situations. The case of TH decaying molecule passes through our consideration with obvious changes. To note some: the rotational recoil shift $\frac{p_\beta^2}{2M_t(1+M_t/M_p)}$ is about half of the T_2 case; the composite recoil shift (13) stays the same. The case of initial nonzero J rotational state leads in final channel to the selection of J rotational states, which causes uniform spectral shift $\sim \frac{(J+1/2)^2}{2MR_e^2}$. Finally, there are shouldn't principal difficulties to make proper modifications caused by the solid state surrounding.

As a conclusion, we can suggest one modification which is easy to incorporate into standard spectrum. It is slight energy dependence of the end-point energy

$$W_0 \Rightarrow W_0 - \frac{W_0 - \epsilon_\beta}{M_t}.$$

This modification is almost irrelevant for the W_0 itself but it can sensibly change final value of m_ν^2 parameter.

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- [5] To be precisely we have to write $\mathbf{q} = \frac{\mathbf{p}_\beta + \mathbf{p}_\nu}{2}$. The simple estimate shows however that neutrino momentum correction is sufficiently small.

FIGURES

FIG. 1. The final states spectrum.

FIG. 2. The absolut difference between spectral sum and its linear approximation for $m_\nu = 1 \text{ eV}$ reference value. The additional line shows $(m_\nu c^2)^4/(W_0 - \epsilon_\beta)$ trend line.



